

CRYSTAL STRUCTURES OF *T. FOETUS* INOSINE MONOPHOSPHATE
DEHYDROGENASE IN COMPLEX WITH SUBSTRATE, COFACTOR AND
ANALOGS AND USES THEREOF

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ABSTRACT OF THE INVENTION

The invention provides a crystalline complex containing *T. foetus* IMPDH in complex with inosine monophosphate (IMP), the complex specified by disclosed
10 atomic coordinates. Also provided are crystalline complexes of containing *T. foetus* IMPDH with both inosine monophosphate (IMP) and mycophenolic acid, with both xanthosine monophosphate (XMP) and mycophenolic acid, with both xanthosine monophosphate (XMP) and nicotinic
15 adenine dinucleotide (NAD), with ribovirin (1- β -D-ribofuranosyl-1,2,4-triazole-3-carboxamide, and with both ribovirin and mycophenolic acid, each complex specified by disclosed atomic coordinates. Also provided by the invention are the atomic coordinates for these complexes.
20 Further provided by the invention are methods for identifying modulations of IMPDH that employ the atomic coordinates of the invention.